



# Scientists create first billion-atom biomolecular simulation

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Researchers at Los Alamos National Laboratory have created the largest simulation to date of an entire gene of DNA, a feat that required one billion atoms to model and will help researchers to better understand and develop cures for diseases like cancer.

“It is important to understand DNA at this level of detail because we want to understand precisely how genes turn on and off,” says Karissa Sanbonmatsu, a structural biologist at Los Alamos. “Knowing how this happens could unlock the secrets to how many diseases occur.”

Modeling genes at the atomistic level is the first step toward creating a complete explanation of how DNA expands and contracts, which controls genetic on/off switching.

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Sanbonmatsu and her team ran the breakthrough simulation on Los Alamos’ Trinity supercomputer, the sixth fastest in the world. The capabilities of Trinity primarily support the National Nuclear Security Administration stockpile stewardship program, which ensures safety, security, and effectiveness of the nation’s nuclear stockpile.

DNA is the blueprint for all living things and holds the genes that encode the structures and activity in the human body. There is enough DNA in the human body to wrap around the earth 2.5 million times, which means it is compacted in a very precise and organized way.

The long, string-like DNA molecule is wound up in a network of tiny, molecular spools. The ways that these spools wind and unwind turn genes on and off. Research into this spool network is known as epigenetics, a new, growing field of science that studies how bodies develop inside the womb and how diseases form.

When DNA is more compacted, genes are turned off and when the DNA expands, genes are turned on. Researchers do not yet understand how or why this happens.

While atomistic model is key to solving the mystery, simulating DNA at this level is no easy task and requires massive computing power.

The Laboratory team partnered with researchers from the RIKEN Center for Computational Science in Japan, the New Mexico Consortium and New York University to collect a large number of different kinds of experimental data and put them together to create an all-atom model that is consistent with that data.

> [Learn more about this research](#)

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